3. Running NCEMSS

Note on Platform dependency:
NCEMSS was originally written for a terminal emulating tektronix 4014 commands. The menus were written to the terminal and the images were displayed on a framestore. The code was executing on a Digital Equipment Corporation microVax II computer under the VMS operating systems. The code has since been ported to other platforms and will run on DEC VMS and Ultrix workstations and on various flavors of Unix running X-windows. However, because of the origin of the program, it still an old style layout dictated by the tektronix terminal. The program uses two windows. One looking like a graphics window displaying push-button style menus and one window for displaying graphics output such as images, diffraction patterns and views of unit cells. The program does not have a modern style interface with a menubar and pull down menus.

NCEMSS is run interactively at a graphics screen using a mouse or other pointing device. The graphics screen may be a a workstation console, an X-window terminal or any computer running as an x-window server. Commands are issued to NCEMSS by moving a cursor to select an appropriate item from a menu. Sometimes, selecting an item from a menu will produce another menu with additional options.

Because of constant changes, the menus mentioned in this manual may not always correspond to the current version of the program for a particular platform. The text will be appropriate for the UNIX version of the program.

3.1 Getting started

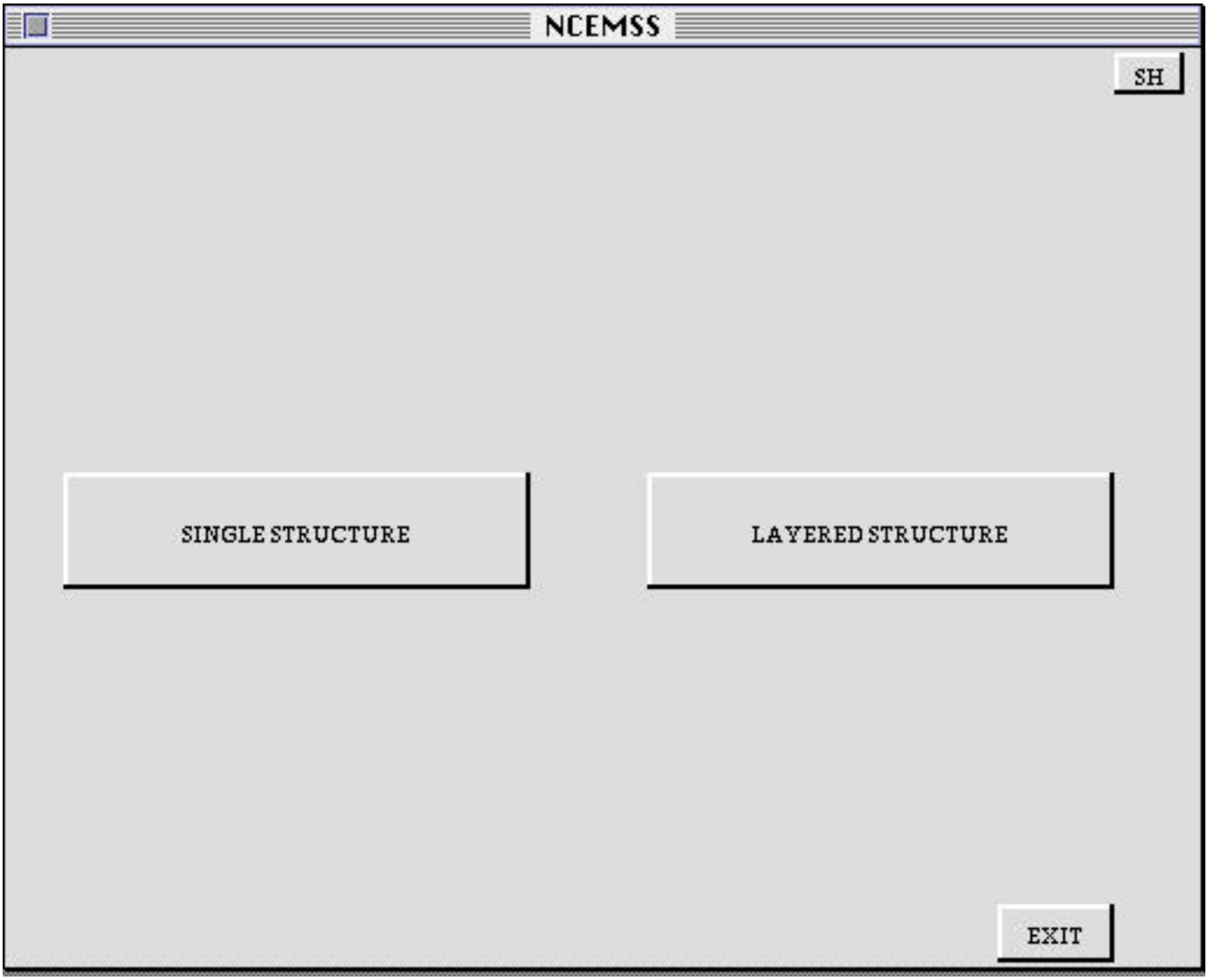
If started from an X-terminal, first type **setenv DISPLAY <IP address>** to set the output to the X-window terminal.

Start NCEMSS by typing **ncemss** followed by a carriage return:

ncemss (return)

this action will produce the SINGLE/LAYERED menu (page 12), by opening two windows on the workstation screen, one being the menu (control) window, the other the image window.

The SINGLE/LAYERED Menu

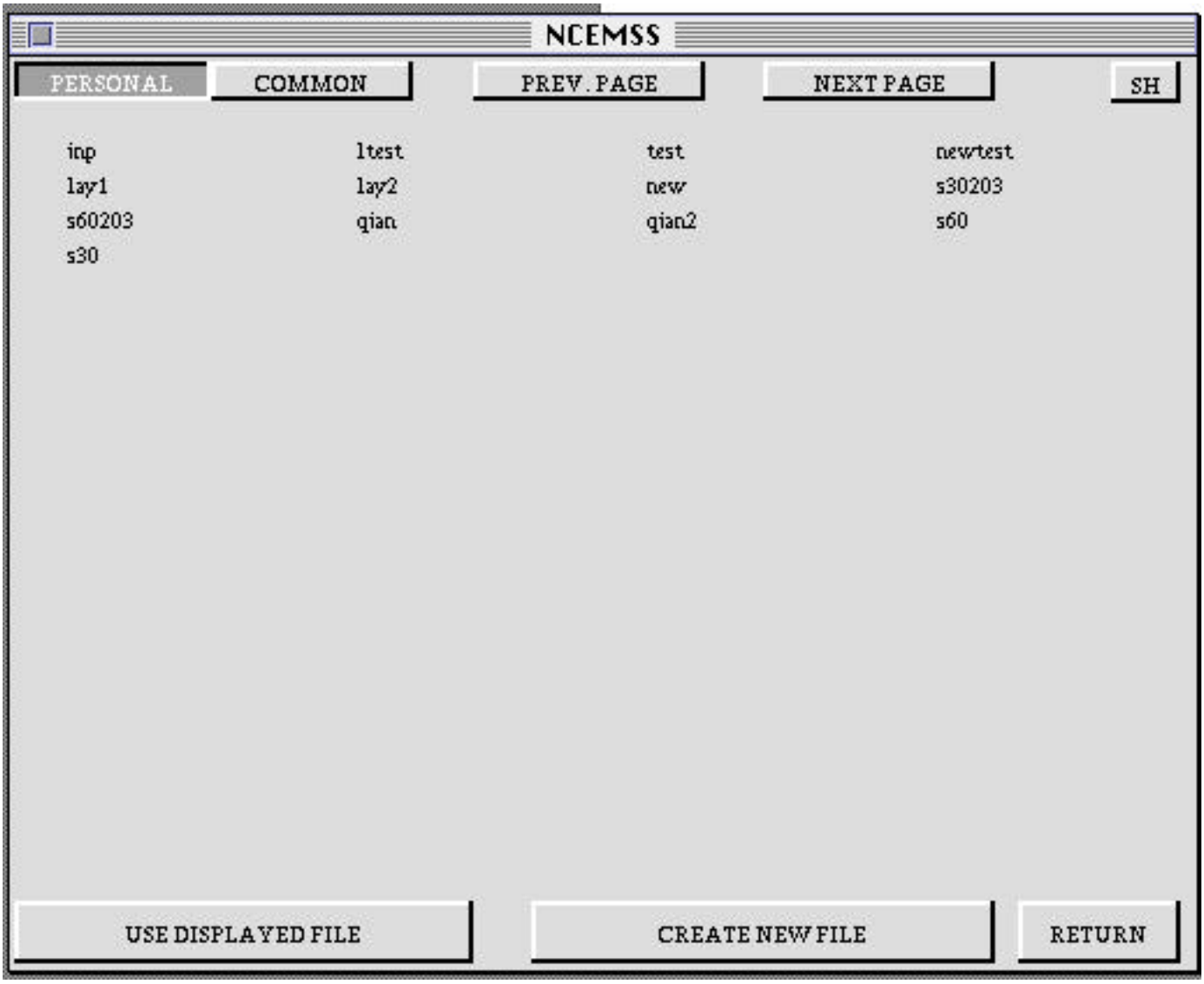


3.2 The SINGLE/LAYERED menu

The first menu encountered by the user on starting to work withNCEMSS consists of three labeled boxes. Any one of these boxes or buttons can be activated by using the mouse to move the screen cursor into the area of the screen within the box, and then pressing the LEFT button on the mouse. At the lower right of the window is the EXIT box, or button. Selecting this box will cause the program to exit and return to the system prompt.

The two major boxes allow the user to specify a choice of either a SINGLE STRUCTURE calculation, or a calculation of the images arising from a LAYERED STRUCTURE. A SINGLE STRUCTURE calculation is one where the specimen structure repeats regularly in thedirection of the electron beam, and is the usual type of image simulation. A LAYERED STRUCTURE calculation is a simulation in which the specimen structure is built up of a number of different structural layers in the electron beam direction, so that the computation requires the use of more than one crystal structure file. Selecting the LAYERED STRUCTURE box produces the SET LAYERS menu (page 46). Selecting SINGLE STRUCTURE produces the FILE-LIST menu (page 14).

The FILE-LIST Menu



3.3 The FILE-LIST menu

The FILE-LIST menu lists the user's structure files on the screen. In addition, there are four boxes across the top of the menu, and three boxes across the bottom. The four top boxes control the listing of the structure names; the right hand pair allow the user to "page" through the list, displaying subsequent pages of structure file names.

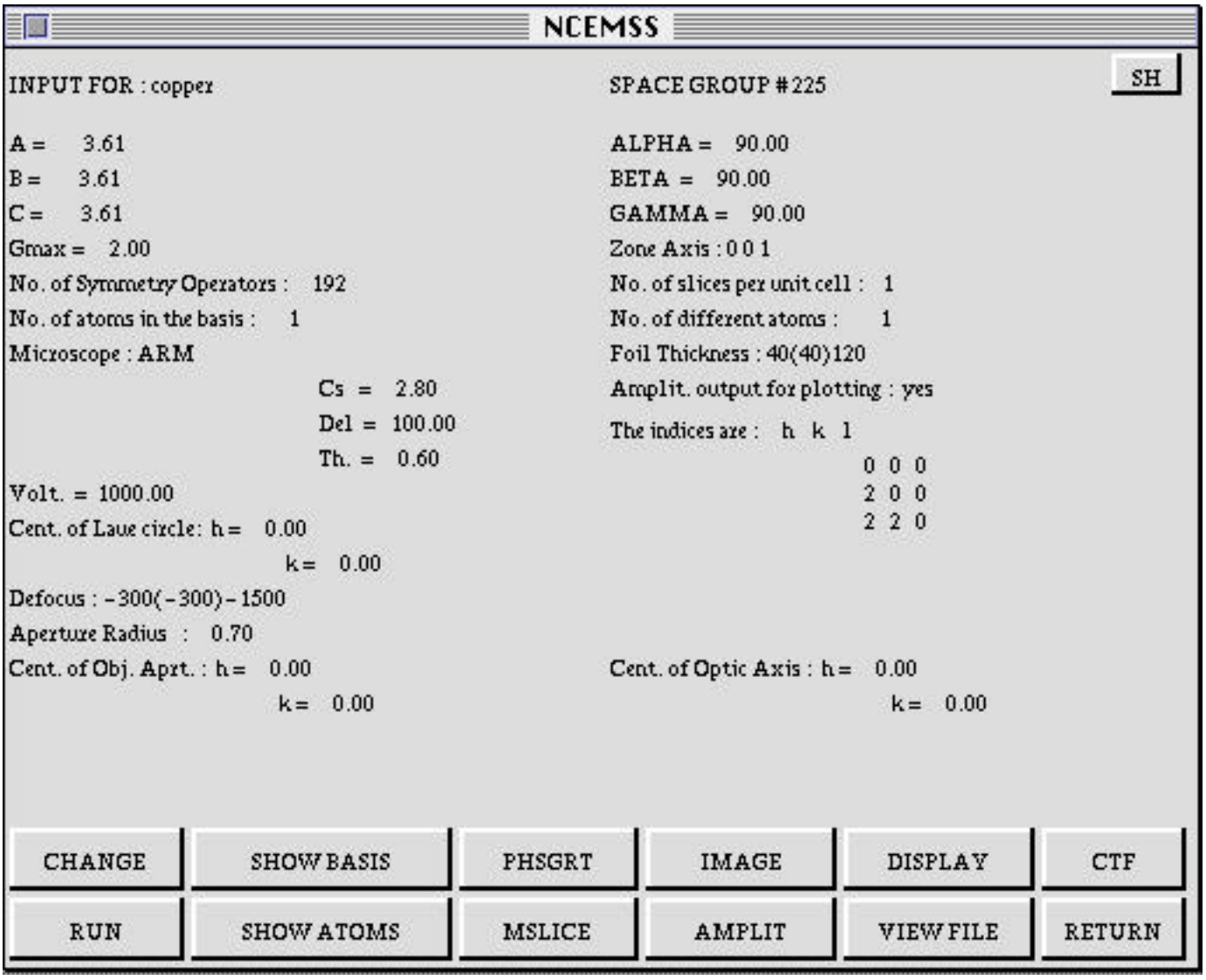
The top left boxes can be used to select lists of files from either the user's PERSONAL collection of structure files, or from a COMMON collection available to all users on the system. The files in the COMMON collection can often serve as useful templates for modification to the user's needs. On entry to the FILE-LIST menu, the PERSONAL box is selected automatically. To obtain the COMMON list, move the cursor to the COMMON box and press the LEFT button on the mouse. To return to your PERSONAL file collection, move the cursor to the PERSONAL box and press the button.

The three boxes at the bottom of the menu are used to proceed from the current menu. The rightmost box is the RETURN box, and is used to go back to the previous menu. Note that many menus have this facility, with the RETURN box situated in the bottom right corner of the menu. The bottom left box is used to notify NCEMSS that the user wishes to use one of the displayed structure files. Moving the cursor to this USE DISPLAYED FILE box and selecting it by clicking the mouse button removes all the other boxes, and allows the user to select one of the displayed files by moving the cursor to the correct filename and clicking the mouse button. Selecting a structure filename causes NCEMSS to read the file and display its parameters in the PARAMETER menu (often referred to as the MAIN or CONTROL menu, because it is the one from which the NCEMSS computation is controlled by the user). The CONTROL menu is shown on page 16.

The CREATE NEW FILE box is selected when the user desires to input a new structural file. Selecting this box with the cursor causes NCEMSS to ask for a unique name for the structure. Entry of the name then produces a PARAMETER menu with no parameter values, and a series of prompts from NCEMSS explaining each parameter needed for input.

HELP: If this is your first use of NCEMSS, it may be helpful to try moving the cursor to each box in turn, asking for the HELP facility by clicking the CENTER button on the mouse as each box is reached. The HELP facility is available for every command box on every menu, and should provide enough information that you will need to consult this Guide only infrequently.

The MAIN Menu



3.4 The PARAMETER or MAIN or CONTROL menu

The main CONTROL menu lists a summary of the control parameters for the current simulation as well as twelve boxes for control of the computation.

When the CREATE NEW FILE option of the FILE-LIST menu (page 14) is selected, an empty PARAMETER menu (with no control boxes) is presented, and NCEMSS prompts for parameters. These parameters have the same form as those presented in the PARAMETER menu when a structure filename is selected from the FILE-LIST menu. When every parameter has been entered, NCEMSS re-presents the PARAMETER menu with the control boxes drawn in and available for use.

3.4.1 Parameters of the PARAMETER menu

INPUT FOR: The parameter displayed next to this prompt is a short title for the structure.

SPACE GROUP #: NCEMSS generates symmetry operators for any one of the 230 space groups, when given the number of the space group required (listed in the International Tables for Crystallography). If the space group required is not one listed in the Tables, a value of zero can be entered.

A, B, C, ALPHA, BETA, GAMMA: These are the unit cell dimensions in Angstrom units, and the unit cell angles in degrees.

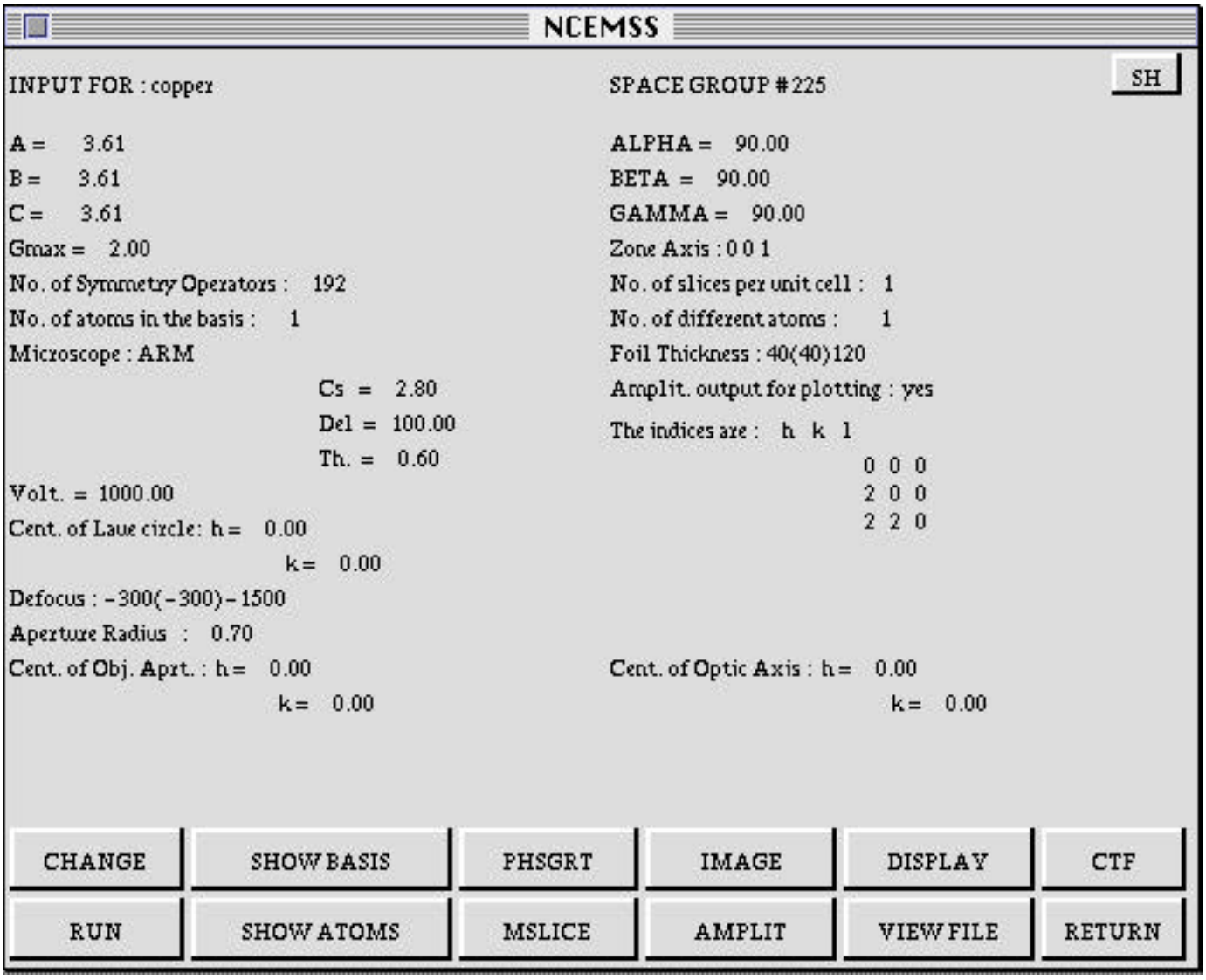
GMAX: The maximum value (in reciprocal Angstrom units) of g to be considered in the multislice diffraction calculation. This value imposes an "aperture" on the diffracted beams included in the dynamic scattering process. It should be large enough to ensure that all significant beam interactions are included. For light atoms and thin crystals, values as low as 2.0 are adequate. For structures with heavy atoms and large crystal thicknesses, values of 3.0 to 4.0 are to be preferred. Note that NCEMSS will compute phase-grating coefficients out to twice GMAX in order to include dynamical interactions correctly (Appendix A).

ZONE AXIS: Specimen orientation is selected by specifying the zone axis desired. Three indices are entered with one space between each.

NO. OF SYMMETRY OPERATORS: If a space group has been selected, the correct value for this parameter will have been entered by NCEMSS. If a value of zero has been entered for the SPACE GROUP #, then the correct number of operators must be entered here.

NO. OF SLICES PER UNIT CELL: For unit cells with large repeat distances in the beam direction, moderate values of GMAX may allow the Ewald sphere to approach the so-called pseudo-upper-layer line that the multislice allows at the reciprocal of the chosen slice thickness. In this case NCEMSS will sub-divide the slice into two or more subslices. How this is done depends upon the potential setting chosen in the SET-UP menu (page 40).

The MAIN Menu



NO. OF ATOMS IN THE BASIS: This value is the number of independent atom positions in the basis or asymmetric unit of the cell. When operated on by the symmetry operators, the basis generates all the atom positions within the cell.

NO. OF DIFFERENT ATOMS: This value is the number of different types of atoms in the specimen structure; difference is due to a different Debye-Waller factor or different atomic number.

MICROSCOPE: The type of electron microscope used to generate the imaging parameters. If a type known to NCEMSS is entered, then NCEMSS provide values for CS, the spherical aberration coefficient of the objective lens (in mm.); DEL, the halfwidth of a Gaussian spread of focus due to chromatic aberration (in Angstrom units); TH., the semi-angle of incident beam convergence (in milliradian). If the type of microscope is unknown to NCEMSS, the above values must be entered seperately (or the data file MICROSCOPES.DAT may be edited to include an appropriate microscope type).

FOIL THICKNESS: The thickness of the specimen foil may be entered as one single number representing the thickness in Angstrom units, or as a series of thicknesses represented by the upper and lower bounds and a thickness step; e.g. 100(50)250 will cause NCEMSS to store the exit wavefield at specimen thicknesses of 100Å to 250Å in steps of 50Å (a total of four thicknesses).

AMPLIT. OUTPUT FOR PLOTTING: A number of diffracted beams may be selected for plotting of their intensity and phase variation as a function of specimen thickness. If YES is answered to the NCEMSS prompt, the number of beams and their indices may be entered.

VOLT.: The electron microscope accelerating voltage in kilovolts.

CENT. OF LAUE CIRCLE: Specimen tilt is specified by entering the center of the Laue circle in units of the h and k indices of the projected two-dimensional reciprocal-space unit cell.

DEFOCUS: The defocus of the objective lens is entered in Ångstrom units with a negative value representing underfocus (weakening of the lens current). As for the FOIL THICKNESS parameter, a single value of defocus may be entered, or a range specified by the upper and lower bounds and the interval; -300(-200)-1100 means defocus values of -300Å, -500Å, -700Å, -900Å and -1100Å.

APERTURE RADIUS: The radius of the objective aperture is specified in reciprocal Ångstrom units.

CENT. OF OBJ. APRT.: The center of the objective aperture is defined in units of the h and k indices of the two-dimensional reciprocal-space unit cell, as for the Laue circle center.

CENT. OF OPTIC AXIS: The center of the optic axis of the electron microscope is specified in terms of the h and k indices of the two-dimensional reciprocal-space unit cell, just as for the Laue circle center and the aperture center.

The MAIN Menu